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<th><strong>Title</strong></th>
<th>Attractive Interaction between Electrons in Semiconductors with Wide Band Gaps by Electron-Photon Interaction</th>
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<tbody>
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Osaka University
Attractive Interaction between Electrons in Semiconductors with Wide Band Gaps by Electron-Photon Interaction

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We theoretically demonstrate attractive interaction between electrons in semiconductors with wide band gaps by electron-photon interaction. At low temperature, wave vectors of electromagnetic waves absorbed in semiconductors with wide band gaps cannot be neglected for those of electron waves, that is, electromagnetic waves affect movements of electrons. Especially, attractive interaction between electrons occurs when one electron changes from a valence band to a conduction band and the other one changes from a conduction band to a valence band, and wide band gaps are necessary in order to obtain effective attractive interaction.

KEYWORDS : attractive interaction, semiconductors with wide band gaps, electron-photon interaction

1. Introduction

In semiconductors, absorption of electromagnetic waves caused by electron-photon interaction has attracted much attention from practical and fundamental viewpoints. This property is used for electronic devices such as lasers and diodes, and provides various valuable applications. A wave vector of electromagnetic waves is approximately $q = 5.07 \times 10^4 [m^{-1}]$ for band gaps approximately $1 [eV]$ in conventional semiconductors, and therefore, $q$ can be neglected for a wave vector of electron waves $k = 4.8 \times 10^8 [m^{-1}]$ at $T=100[K]$.

Recently, however, semiconductors with wide band gaps have been reported from experimental and theoretical viewpoints. For example, AlN ($E_g=6.2 [eV]$) and KBeF$_3$ ($E_g=8.1[eV]$) are reported experimentally and theoretically, respectively.\(^1\,\text{,}\,\text{2}\)
When $E_g=10[eV]$ is considered, a wave vector of electromagnetic waves is approximately $q = 5.07 \times 10^7 [m^{-1}]$. Therefore, $q$ cannot be neglected for a wave vector of electron waves, $k = 4.8 \times 10^7 [m^{-1}]$ at $T=1[K]$, and we must consider effects of the electromagnetic waves on movements of electron waves.

In this paper, therefore, we investigate electron-photon interaction in semiconductors with wide band gaps at low temperature in considering the effects of wave vectors of electromagnetic waves on those of electron waves. This interaction is similar to electron-phonon interaction, since photons and phonons are both bosons. The electron-phonon interaction causes attractive interaction between electrons, and therefore, we can expect attractive interaction by the electron-photon interaction. We theoretically demonstrate the electron-photon interaction by the same method as used in the electron-phonon interaction.

2. Nonperturbation and perturbation Hamiltonians of electron-photon interaction

By using creation and annihilation operators, a vector potential of electromagnetic waves is represented as follows.

$$A(r) = \frac{1}{2} \sum_{q,\lambda} \left( A_{q,\lambda} e_{q,\lambda} a_{q,\lambda} \exp(iq \cdot r) + A^{*}_{-q,\lambda} e_{-q,\lambda} a^{+}_{-q,\lambda} \exp(-iq \cdot r) \right)$$

$$= \frac{1}{2} \sum_{q,\lambda} \left( A_{q,\lambda} e_{q,\lambda} a_{q,\lambda} + A^{*}_{-q,\lambda} e_{-q,\lambda} a^{+}_{-q,\lambda} \right) \exp(iq \cdot r)$$

$$= \frac{1}{2} \sum_{q,\lambda} A_{q,\lambda} \left( a_{q,\lambda} + a^{+}_{-q,\lambda} \right) \exp(iq \cdot r)$$

$$\text{(1)}$$

where

$$A_{q,\lambda} = \frac{\sqrt{2\eta}}{\sqrt{\epsilon \Omega \omega_\lambda}}$$

$$\text{(2)}$$

$q$ and $\lambda$ indicate a wave vector and one of two polarizations of electromagnetic waves. $A_{q,\lambda}$ and $e_{q,\lambda}$ are a coefficient and a polarized unit vector of a vector potential, respectively. $a_{q,\lambda}$ and $a^{+}_{q,\lambda}$ are annihilation and creation operators of electromagnetic waves, respectively. $\epsilon$, $\Omega$ and $\omega_\lambda$ are the dielectric index, a volume of crystals and a frequency of electromagnetic waves, respectively. $A(r)$ is assumed to satisfy the Coulomb gauge, $\nabla \cdot A(r) = 0$.

In the existence of the vector potential, the energy of electrons is

$$\left\{ p(r) + eA(r) \right\}^2$$

$$\frac{2m}{2m}$$

$$= \frac{p^2(r)}{2m} + \frac{e}{2m} \left\{ A(r) \cdot p(r) + p(r) \cdot A(r) \right\}$$

$$+ \frac{e^2 A^2(r)}{2m}$$

$$= \frac{p^2(r)}{2m} + \frac{e}{m} A(r) \cdot p(r) + \frac{e^2 A^2(r)}{2m} \text{ (3)}$$

$$\text{(3)}$$

$$\text{(3)}$$

That is, the second term in Eq. (3) is the interaction term.

The nonperturbation Hamiltonian is

$$H_0 = H_{electron} + H_{photon}$$

$$= \sum_{i=0,1} \sum_{k,\sigma} \varepsilon^{(i)}_k c_{k,\sigma}^{(i)} + \sum_{q,\lambda} \eta q A_{q,\lambda} a_{q,\lambda}$$

$$\text{(4)}$$

$$\text{(4)}$$

$H_{electron}$ and $H_{photon}$ are Hamiltonians of electrons and photons, respectively. $k$ and $\sigma$ are a wave vector and a spin of electrons. $c^{(i)}_{k,\sigma}$ and $c^{(i)*}_{k,\sigma}$ are annihilation and creation operators of electrons, respectively. $\varepsilon^{(i)}_k$ is an energy of electrons. $c$ and $\sigma$ indicate conduction and valence bands, respectively.

By Bloch’s theorem, the wave function of
Attractive Interaction between Electrons in Semiconductors with Wide Band Gaps by Electron-Photon Interaction

The interaction Hamiltonian is represented as follows.

\[ H_{\text{int}} = H_{\text{electron-photon}} \]

\[ = \int dr \psi^\dagger(r) \frac{e}{m} A(r) \cdot p(r) \psi(r) \]

\[ = \sum_{i,j} \sum_{k,\sigma} \sum_{q,\alpha} \sum_{k',\sigma'} \frac{e}{2m} A_{q,\alpha} \]

\[ \times c_{k',\sigma'}^{(j)} (a_{q,\alpha} + a_{q,\alpha}^\dagger) c_{k,\sigma}^{(i)} \]

\[ = \int dr \exp \{i(-k'+k + q) \cdot r\} \]

\[ \times u_{k',\sigma'}^{(j)} (r) \psi_{q,\alpha} \cdot \{p(r) + \eta k \} \psi_{k,\sigma}^{(i)} (r) \]

\[ = \int dr u_{k',\sigma'}^{(j)} (r) e_{q,\alpha} \cdot \{p(r) + \eta k \} u_{k,\sigma}^{(i)} (r) \]

\[ \approx \int dr u_{k',\sigma'}^{(j)} (r) e_{q,\alpha} \cdot \{p(r) + \eta k \} u_{k,\sigma}^{(i)} (r) \]

\[ = \int dr u_{k',\sigma'}^{(j)} (r) e_{q,\alpha} \cdot \{p(r) + \eta k \} u_{k,\sigma}^{(i)} (r) \]

\[ = \langle j | e_{q,\alpha} \cdot \{p(r) + \eta k \} \delta_{i,j} \rangle \]

\[ + \langle j | e_{q,\alpha} \cdot \{p(r) + \eta k \} \delta_{i,j} \rangle \]

\[ \delta_{i,j} \text{ is Kronecker's delta. For simplicity, we neglected dependences of } u_{k,\sigma}^{(i)} \text{ on } k \text{ and } \sigma, \text{ as considering absorption of electromagnetic waves in conventional semiconductors. The first term in Eq. (7) is zero when } i = j, \text{ while the second term in Eq. (7) is zero when } i \neq j. \text{ Therefore, } H_{\text{int}} \text{ is represented as follows.} \]

\[ H_{\text{int}} = \sum_{i,j} \sum_{k,\sigma} \sum_{q,\alpha} \sum_{k',\sigma'} D_{k,\sigma,q,\alpha}^{(i)} c_{k,q,\alpha}^{(i)} (a_{q,\alpha} + a_{q,\alpha}^\dagger) c_{k,\sigma}^{(i)} \]

\[ , \text{ where} \]

\[ D_{k,\sigma,q,\alpha}^{(i)} = \frac{e A_{q,\alpha} M_{k,\sigma,q,\alpha}^{(i)}}{2m} \]

This interaction Hamiltonian is similar to that of electron-phonon interaction although \( D_{k,\sigma,q,\alpha}^{(i)} \) is independent of \( k \) in the electron-phonon interaction, differently from the electron-photon interaction.

3. Effective electron-photon interaction

The Hamiltonian of electron-photon interaction is represented as follows.

\[ H = H_0 + H_{\text{int}} \]

By the method used in electron-phonon interaction, we obtain the following effective Hamiltonian.

\[ \Rightarrow e^{-S} H e^S \]

\[ = H_0 + \frac{1}{2} [H_{\text{int}}, S] + O(S^3) \]

\[ \text{, where} \]

\[ H_{\text{int}} = [S, H_0] \]

By Eq. (12), the following equations are obtained.

\[ \langle q, \lambda | S | 0 \rangle = \sum_{i,j} \sum_{k,\sigma} D_{k,\sigma,q,\alpha}^{(i)} c_{k,q,\alpha}^{(i)} c_{k,\sigma}^{(i)} \]

\[ \langle S | q, \lambda \rangle = \sum_{i,j} \sum_{k,\sigma} D_{k,\sigma,q,\alpha}^{(i)} c_{k,q,\alpha}^{(i)} c_{k,\sigma}^{(i)} \]

Moreover, the following equations are obtained from \( H_{\text{int}} \).

\[ \langle q, \lambda | H_{\text{int}} | 0 \rangle = \sum_{i,j} \sum_{k,\sigma} D_{k,\sigma,q,\alpha}^{(i)} c_{k,q,\alpha}^{(i)} c_{k,\sigma}^{(i)} \]
The second term in Eq. (11) corresponds to the effective electron-photon interaction. From Eqs. (12)-(16), electron correlation by electron-photon interaction is obtained.

\[ H_{\text{eff}} = \frac{1}{2} \langle 0 | [H_{\text{int}}, S] | 0 \rangle \]

\[ = \frac{1}{2} \langle 0 | H_{\text{int}} S - S H_{\text{int}} | 0 \rangle \]

\[ = \frac{1}{2} \sum_{q, \lambda} \langle 0 | H_{\text{int}} q, \lambda | q, \lambda | S | 0 \rangle \]

\[ - \langle 0 | S q, \lambda | q, \lambda | H_{\text{int}} | 0 \rangle \}

\[ = \frac{1}{2} \sum_{i,j} \sum_{q, \lambda} \sum_{k, \sigma} \sum_{q, \sigma} D_{ij}^{(q),q,\lambda} D_{ij}^{(q),q,\lambda} \]

\[ \times \left\{ \frac{1}{\varepsilon_{k}^{(i)} - \varepsilon_{k}^{(j)} - \eta \omega_{q}} \right\}

\[ - \frac{1}{\varepsilon_{k}^{(i)} - \varepsilon_{k}^{(j)} + \eta \omega_{q}} \}

\[ \times c_{k,\sigma}^{(i)} c_{k,\sigma}^{(j)} c_{k,q,\sigma}^{(i)} c_{k,q,\sigma}^{(j)} \]

\[ = \frac{1}{4} \sum_{i,j} \sum_{q, \lambda} \sum_{k, \sigma} \sum_{q, \sigma} D_{ij}^{(q),q,\lambda} D_{ij}^{(q),q,\lambda} \]

\[ \times \left\{ \frac{1}{\varepsilon_{k}^{(i)} - \varepsilon_{k}^{(j)} - \eta \omega_{q}} \right\}

\[ - \frac{1}{\varepsilon_{k}^{(i)} - \varepsilon_{k}^{(j)} + \eta \omega_{q}} \}

\[ \times c_{k,\sigma}^{(i)} c_{k,\sigma}^{(j)} c_{k,q,\sigma}^{(i)} c_{k,q,\sigma}^{(j)} \]

\[ + (q \rightarrow -q) \]

\[ = -\frac{1}{2} \sum_{i,j} \sum_{q, \lambda} \sum_{k, \sigma} \sum_{q, \sigma} D_{ij}^{(q),q,\lambda} D_{ij}^{(q),q,\lambda} \]

\[ \times \left\{ \frac{\eta \omega_{q}}{\eta \omega_{q} - (\varepsilon_{k}^{(i)} - \varepsilon_{k}^{(j)} - \eta \omega_{q})} \right\}

\[ + \frac{\eta \omega_{q}}{\eta \omega_{q} - (\varepsilon_{k}^{(i)} - \varepsilon_{k}^{(j)} + \eta \omega_{q})} \}

\[ \times c_{k,\sigma}^{(i)} c_{k,\sigma}^{(j)} c_{k,q,\sigma}^{(i)} c_{k,q,\sigma}^{(j)} \]

\[ (q \rightarrow -q) \]

\[ \text{depends on } k \text{ and } k' \text{ whether } H_{\text{eff}} \text{ is attractive or repulsive. Therefore, sums of such interaction become very small. When } i \neq j \text{ and } i' \neq j', \text{ on the other hand, } D_{ij}^{(q),q,\lambda} 	ext{ and } D_{ij}^{(q),q,\lambda} \text{ are independent of } k \text{ and } k'. \]

\[ \text{When } i = i' \text{ and } j = j', \]

\[ D_{ij}^{(q),q,\lambda} D_{ij}^{(q),q,\lambda} \]

\[ = \left( \frac{e}{2m} \right)^2 A_{q,\lambda} \langle j | e_{q,\lambda} \cdot p(r) | i \rangle \]

\[ A_{q,\lambda} \langle j | e_{q,\lambda} \cdot p(r) | i \rangle \]

\[ = \left( \frac{e}{2m} \right)^2 | A_{q,\lambda} |^2 \langle j | e_{q,\lambda} \cdot p(r) | i \rangle \]

\[ \langle j | e_{q,\lambda} \cdot p(r) | i \rangle \]

\[ \text{It depends on } u^{(i)} \text{ and } u^{(j)} \text{ whether this term is attractive or repulsive. When } i = j' \text{ and } j = i', \]

\[ D_{ij}^{(q),q,\lambda} D_{ij}^{(q),q,\lambda} \]

\[ = \left( \frac{e}{2m} \right)^2 A_{q,\lambda} \langle j | e_{q,\lambda} \cdot p(r) | j \rangle \]

\[ A_{q,\lambda} \langle j | e_{q,\lambda} \cdot p(r) | j \rangle \]

\[ = \left( \frac{e}{2m} \right)^2 | A_{q,\lambda} |^2 \langle j | e_{q,\lambda} \cdot p(r) | j \rangle \]

\[ \langle j | e_{q,\lambda} \cdot p(r) | j \rangle \]

\[ = \left( \frac{e}{2m} \right)^2 | A_{q,\lambda} |^2 \langle j | e_{q,\lambda} \cdot p(r) | j \rangle |^2 \geq 0. \]

This term is positive regardless of k, u^{(i)} and u^{(j)}, and we focus our attention only on this interaction. Then, the electron correlation is represented as follows.
Attractive Interaction between Electrons in Semiconductors with Wide Band Gaps by Elect

\[ H_{\text{eff}} = -\frac{1}{2} \sum_{i,j} \sum_{k,\sigma} \sum_{\eta,\lambda} \left( \frac{e}{2m} \right)^2 \times A_{q,\lambda}^2 \left| i | e_{q,\lambda} \cdot p(r) j \right|^2 \times \left\{ \frac{\eta \omega_q}{(\eta \omega_q)^2 - (\epsilon_k^{(i)} - \epsilon_{k,q}^{(j)})^2} \right\} \left\{ \frac{\eta \omega_q}{(\eta \omega_q)^2 - (\epsilon_k^{(i)} - \epsilon_{k,q}^{(j)})^2} \right\} \times c_{k+q,\sigma}^{(i)} c_{k,q,\sigma}^{(j)} c_{k,\sigma}^{(i)} c_{k,\sigma}^{(j)} \]

(20)

This interaction occurs when one electron changes from a valence band to a conduction band and the other one changes from a conduction band to a valence band. Since electrons near band gaps affect electronic properties, \((\epsilon_k^{(i)} - \epsilon_{k,q}^{(j)})^2 \approx E_g^2\) is satisfied. Moreover,

\[
\left\langle i | e_{q,\lambda} \cdot p(r) j \right\rangle \\
= \frac{i m}{\eta} \left\langle \epsilon^{(j)} - \epsilon^{(i)} \right\rangle \left\langle i | e_{q,\lambda} \cdot r j \right\rangle \\
= \pm \frac{i m}{\eta} E_g \left\langle i | e_{q,\lambda} \cdot r j \right\rangle. 
\]

(21)

By inserting Eqs. (2) and (21) into Eq. (20),

\[ H_{\text{eff}} = -\sum_{i,j} \sum_{k,\sigma} \sum_{\eta,\lambda} V_{\text{electron–photon}} \times c_{k+q,\sigma}^{(i)} c_{k,q,\sigma}^{(j)} c_{k,\sigma}^{(i)} c_{k,\sigma}^{(j)} \]

(22)

where

\[ V_{\text{electron–photon}} = \frac{1}{2} \left( \frac{e}{2m} \right)^2 \times \left| A_{q,\lambda}^2 \right|^2 \left| i | e_{q,\lambda} \cdot p(r) j \right|^2 \times \left\{ \frac{\eta \omega_q}{(\eta \omega_q)^2 - (\epsilon_k^{(i)} - \epsilon_{k,q}^{(j)})^2} \right\} \left\{ \frac{\eta \omega_q}{(\eta \omega_q)^2 - (\epsilon_k^{(i)} - \epsilon_{k,q}^{(j)})^2} \right\} \times c_{k+q,\sigma}^{(i)} c_{k,q,\sigma}^{(j)} c_{k,\sigma}^{(i)} c_{k,\sigma}^{(j)} \]

(23)

When \(\eta \omega_q > E_g\), the electron-photon interaction is attractive. When \(\eta \omega_q \gg E_g\), however, \(V_{\text{electron–photon}}\) becomes small, and effective attractive interaction cannot be obtained. In order to obtain effective attractive interaction, therefore, semiconductors with wide band gaps are necessary for \(\eta \omega_q \approx 10(eV)\).

If the interaction, which occurs when one electron changes from a valence band to a conduction band and the other one changes from a conduction band to a valence band, is main in semiconductors with wide band gaps, and exceeds the Coulomb interaction, the attractive interaction may cause Cooper pairs. As is well known, Cooper pairs have attracted great interest since superconductivity can be explained by attractive interaction of electrons.

4. Conclusion

We theoretically demonstrated attractive interaction between electrons in semiconductors with wide band gaps by electron-photon interaction. The attractive interaction occurs when one electron changes from a valence band to a conduction band and the other one changes from a conduction band to a valence band, and wide band gaps are necessary in order to obtain effective attractive interaction.

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References


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